

The 16th International Conference on X-ray Absorption Fine Structure (XAFS16)

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Abstract. This preface of the proceedings volume of the 16th International Conference on X-ray Absorption Fine Structure (XAFS16) gives a glance on the five days of cutting-edge X-ray science which were held in Karlsruhe, Germany, August 23 – 28, 2015. In addition, several satellite meetings took place in Hamburg, Berlin and Stuttgart, a Sino-German workshop, three data analysis tutorials as well as special symposia on industrial catalysis and XFELs were held at the conference venue.

1. Preface

The 16th International Conference on X-ray Absorption Fine Structure (XAFS16 - www.xafs16.org) was held at the Karlsruhe Institute of Technology (KIT) in Karlsruhe, Germany, from 23rd to 28th August 2015. More than 550 participants - including more than 160 early career scientists - from 37 countries all around the world attended this important event which took place, appropriately, in the UNESCO “International Year of Light and Light-based Technologies” (<http://www.light2015.org/>). At the same time, the XAFS16 host city Karlsruhe celebrated the 300th anniversary of its foundation by Margrave Karl Wilhelm of Baden-Durlach in 1715, a birthday commemorated with spectacular events like the “Schlosslichtspiele” throughout the town center (Figure 1), which many of the participants attended.

Since the first XAFS meeting in 1981 in Daresbury, UK, the XAFS conference series has become the foremost international meeting covering developments and applications in X-ray absorption spectroscopy and related techniques. The preceding conferences took place in Stanford in 2006 [1], Camerino in 2009 [2] and Beijing in 2012 [3]. The last and up to now only XAFS conference in Germany was XAFS8, held in Berlin in 1994. Jointly organized by KIT (Karlsruhe), DESY (Hamburg), HZB (Berlin) and the European XFEL (Hamburg) and under the auspices of the International X-ray Absorption Society (IXAS), XAFS16 attracted a new record number of participants (Figure 2). The local organization was provided by the KIT institutes IBPT, INE, IKFT, ITCP and the ANKA synchrotron facility, with Professor Jan-Dierk Grunwaldt chairing the local organizing committee.





Figure 1. Illumination of the façade of Karlsruhe’s palace at the heart of the town center during the “Schlosslichtspiele” in summer 2015. The installation symbolizes the discovery of electromagnetic waves (1886) by Heinrich Hertz in Karlsruhe at the Technische Hochschule, a predecessor of today’s KIT (Copyright: Karlsruhe | Tourismus).

The symposia and accompanying poster sessions addressed virtually all aspects of X-ray absorption spectroscopy – from the latest theoretical developments to instrumentation and applications – covering topics from the in-situ characterization of catalytic reaction processes, environmental contaminant and radionuclide speciation, to novel developments in medical applications and forensic analysis of cultural and historical objects. Altogether 9 plenary lectures, 26 keynotes and almost 200 contributed talks were presented at the conference in 18 different topics (cf. section 3) grouped in 9 scientific fields - starting with field I ‘*Theory, modelling and data analysis*’. In the development of XAFS theory a gradual transition from semi-empirical codes to first principle codes is being observed, also encompassing the metal L-edges. Data analysis is at the heart of all XAFS techniques and, apart from the hands-on courses and the satellite meeting ‘*Data acquisition, treatment, storage - quality assurance in XAFS spectroscopy*’, XAFS data treatment and modelling was the topic of several invited and contributed talks at the conference. In field II ‘*New sources and new instrumentation*’ the status of numerous existing and newly established synchrotron beamlines was covered (cf. several contributions in these proceedings) - the trend is towards faster measurements, specialized beamlines (e.g., for catalysis, energy or radionuclide research), new detectors or detectors that operate at room temperature, to name a few examples. A further prominent trend is towards spatial resolution, even into the 5 – 10 nm regime, and unprecedented energy resolution with high energy fluorescence detected XAS and X-ray emission spectroscopy. While XFELs definitely develop towards an interesting source, pushing the frontiers of the XAFS technique at large scale accelerator facilities (as demonstrated in a dedicated workshop at the conference), an equally challenging and promising trend was also observed: the development of competitive laboratory XAS and XES instrumentation based on X-ray tubes or plasma sources. The trends in field III ‘*Advanced methods*’ were strongly connected to the previous fields: X-ray emission (XES) and valence-to-core (VTC) emission spectroscopy was already one topic highlighted in the first plenary talk by Serena de Beer on the nitrogenase enzyme, and continued through many talks focusing on resonant and non-resonant XES applications. In particular the recent improvements of the underlying theory have made XES a powerful hard X-ray probe with impact in many areas, like field IV ‘*Chemistry, catalysis, operando and time-resolved studies*’, where in situ and operando studies were reported in vast broadness. Sophisticated high

energy resolution methods such as high energy resolved fluorescence detected (HERFD) or partial fluorescence yield (PFY) XANES are meanwhile applied in other fields such as radionuclide and earth and environmental research (field V), e.g., for the study of transient or minority oxidation states in mixed valence actinide systems, or for the investigation of the mobility and bioaccumulation of heavy metal contaminants such as mercury, as illustrated in the plenary lecture given by Alain Manceau.

There was a substantial number of materials science studies submitted to XAFS16, which were split into the separate fields related to the ‘*Science of materials*’ (VI) and ‘*Energy-related materials*’ (VII). In this context, not only studies highlighting structure-property relationships were presented, but also exciting operando studies on batteries and energy storage materials. The broadness of the XAFS application field was further demonstrated with plenary lectures, keynote and contributed talks in the field of ‘*Biology and soft matter*’ (VIII). Last but not least, a special session on spatially resolved XAS and X-ray microscopy (field IX: ‘*Microscopy, beamlines, applications, cultural heritage*’) gave an excellent overview of the dynamic developments in this area. Microscopy is now conducted on all length scales from the μm (or even mm/cm) to the 50 nanometer range. Although ptychography offers new opportunities, achieving X-ray absorption spectroscopy contrast at the ultimate 5 nm scale remains a wish not yet fulfilled. Finally, the important role that X-ray absorption spectroscopy has traditionally played in the commercial use of synchrotrons and for industrial research was reflected in a special symposium dedicated to current and potential applications in industrial XAFS research.



Figure 2. The official conference photo (Copyright: Carina Braun | KIT) taken at the site of the old stadium, KIT Campus South. The inset shows the conference logo designed by Wilfrid Schroeder, KIT († 2015).

In addition to the main conference a number of satellite meetings covering specialist topics were held at HZB (20 - 21 August 2015, ‘*Time and energy-resolved soft X-ray spectroscopy*’, organized by Emad Flear Aziz), at DESY (21 - 22 August 2015, ‘*Data acquisition, treatment, storage and quality assurance in XAFS spectroscopy*’, organized by Edmund Welter), and at the MPI-IS in Stuttgart (30 August – 2 September 2015, ‘*Application of XAFS to the study of magnetic materials*’, organized by Eberhard Goering). Moreover, a Sino-German Workshop on ‘*In situ Spectroscopy on Catalysis and Membranes*’ at KIT (August 28 – 29, 2015, organized by Ying Zhou, Andreas Goldbach and Jan-Dierk Grunwaldt), and three data analysis tutorials coordinated by Federico Benzi at KIT on FEFF9 (August 23, 2015, John Rehr), GNXAS (August 23, 2015, Andrea Di Cicco) and CTM4XAS (August 29, 2015, Frank de Groot) were held.

The International X-ray Absorption Society (IXAS) used the occasion of the XAFS16 conference to honour a number of scientists whose activities have contributed to the continued development of X-ray absorption spectroscopy: the Edward Stern Prize was awarded jointly to Majed Chergui, Professor of Physics and Chemistry at EPFL Lausanne, Switzerland (for his pioneering work in the field of time-resolved X-ray absorption spectroscopy) and Andrea Di Cicco, Professor of Physics at the Università di Camerino, Italy (for outstanding achievements and pioneering work in the application of XAS to disordered systems). Dr. Amélie Juhin of the French National Centre for Scientific Research in Paris received the Farrel Lytle Prize for her contribution to the understanding of X-ray dichroism and resonant inelastic X-ray scattering, and the Dale Sayers Prize for outstanding young scientists went to Dr. Narcizo Souza-Neto, beamline scientist at the Brazilian Synchrotron Light Laboratory in Campinas, for the development of instrumentation for the use of synchrotron techniques under extreme conditions, such as high pressures (Figure 3).

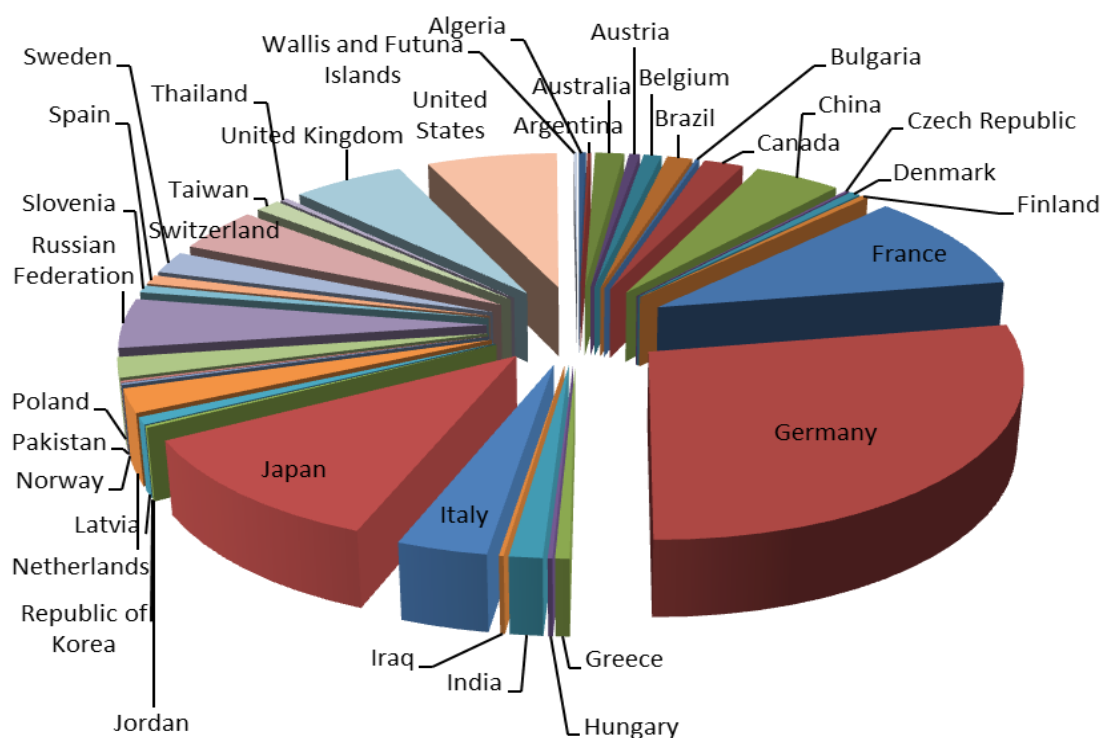


Figure 3. The prize-winners together with the conference organizers - from left to right: Pieter Glatzel, new IXAS chairman, Bruce Bunker, former IXAS chairman, Andrea Di Cicco, Majed Chergui, Amélie Juhin, Narcizo Souza-Neto, and XAFS16 chairman Jan-Dierk Grunwaldt (Copyright: Carina Braun | KIT).

The social program of XAFS16 encompassed excursions to attractive locations near Karlsruhe - a guided walking tour of Heidelberg's old town and castle, a wine tasting tour of the Affentaler cellars in Bühl near Baden-Baden and a visit of the medieval Maulbronn Monastery, one of Germany's UNESCO world heritage sites. The conference banquet was held at the Center of Art and Media (ZKM) in Karlsruhe, a worldwide renowned institution for computer based art and media design. The dinner was preceded by a tour of the 'Global Games' exhibition at ZKM, a hands-on exhibition of the developments in the area of computer games during the past decades.

At the conclusion of the conference the participants had the opportunity to visit the ANKA synchrotron radiation facility at KIT Campus North, with currently three beamlines dedicated to X-ray spectroscopy and where the CAT-ACT beamline for catalyst and actinide research is currently being commissioned. In the closing presentations the hosts of the next conference, XAFS17 (www.xafs2018.com), which will take place in Krakow, Poland in 2018 were introduced. We look forward to meet many of the XAFS16 attendees at this occasion!

2. Nationality of XAFS16 conference attendees



3. Original list of topics offered for abstract submission

The following topics were grouped by nine program committees into scientific fields I - IX for refereeing and setting up the time schedule of the conference:

1. X-ray facilities, instrumentation, optics
2. Materials science and energy-related materials
3. Catalysis
4. Radioactive and nuclear materials
5. Life science, biology and biochemistry
6. Earth and environmental sciences
7. Cultural heritage
8. Atoms and molecules
9. Nanotechnology
10. Surfaces and interfaces
11. Magnetism
12. Soft matter
13. X-ray scattering and electron spectroscopy (XES, RIXS, NIXS, HERFD, and XPS)
14. Theoretical methods
15. Software, data analysis
16. New methods and combination of techniques
17. Spectroscopies at XFEL sources, time-resolved and ultrafast techniques
18. X-ray microscopy

4. Committees, scientific sessions and staff

We would like to thank the members of the International Advisory Committee, the Program Committee and all reviewers evaluating more than 600 original abstracts submitted to the conference and the manuscripts collected in this *J. Phys.: Conf. Ser.* proceedings volume from the XAFS16 conference and the satellite meeting in Hamburg for their dedication and invaluable effort! Many of them have served in chairing the scientific sessions of the many different topics and setting up the program in 9 fields. Melissa A. Denecke is especially acknowledged for organizing and chairing the poster award committee.

Chairman of the Conference:

Jan-Dierk Grunwaldt

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References

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